Kerogen texture modeling, adsorption and transport properties

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Organic shale are an heterogeneous multiscale materials made of sedimentary rocks composed of organic mater inclusions called kerogen. These inclusions ranging from the nano to the micrometer size and are a key component in hydrocarbon production. During burial, increase of temperature (T) and pressure (P) initiate kerogen degradation, that originate hydrocarbon molecules. Molecules are trapped into the complex pore network of kerogen, ranging from subnano to the micrometer size. At the early stage of maturation, immature kerogen produce long molecules corresponding to shale-oil, while at a late maturation stage, hydrocarbon are cracked and transformed in small molecules corresponding to the gaz. Physical and chemical properties of trapped hydrocarbons mixture (from 1 to few tens CHx groups) into multiscale porous system are still poorly understood.
In order to study these systems, we have built atomistic structure of kerogen, generated from experimental data. Nanoporous kerogen was first generated by reverse Monte Carlo technique based on the neutron diffraction spectrum [1], while mesoporosity is included from tomography data of kerogen samples [2].
We first evidenced by Grand Canonical Monte Carlo simulations [3] a selective or reverse selective adsorption, depending on chain lengths, pore diameters and the thermodynamical conditions of kerogen. At low T, adsorption of long chains are favored in small pores, while at high T, adsorption of long chains are favored in large pores. This behavior come from a competition between adsorption energy of the confined fluid and molecules conformational entropy. These results are important about diffusion. Indeed, at small pore size, diffusion is mainly driven by the fluid/wall adsorption. Thus, depending on the thermodynamical conditions fluid diffusion follow a selective or reverse selective diffusion for small thermodynamical conditions change. In this work, we connect thermodynamical behaviors to diffusion behaviors and we show the complex interplay between the kerogen texture, chemical nature of the fluid, thermodynamics and diffusion at small scale.

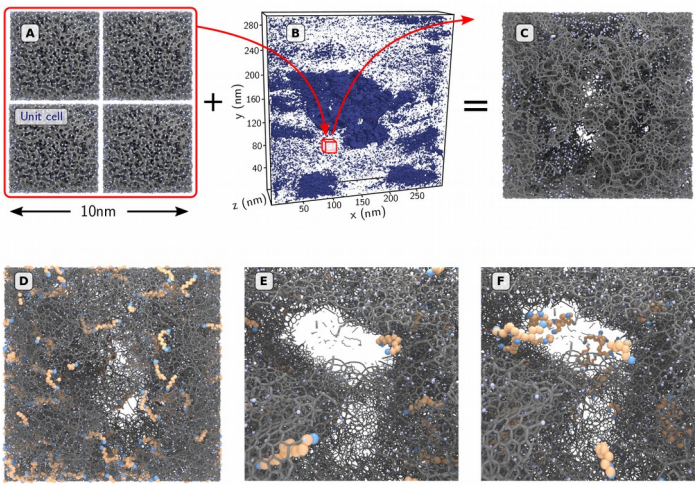

Figure 1. *A) Duplicated nanoporous kerogen structure generated by reverse hybrid Monte Carlo simulations from neutron diffraction scattering. B) Tomography mapping of kerogen structure. C) Atomistic kerogen structure embedded experimental nanoporosity and experimental mesoporosity. D) Adsorption of dodecane molecules into multiscale porous kerogen. E) At low T and low P, adsorption takes place in the nanoporosity of the structure remaining a void mesopore. This behavior correspond to a selective adsorption of the fluid into small pores. F) At high T and low P, molecule previously locate in small pores desorbed and populate the mesopore.*

References

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